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E Hodzic[1], G Esmaeelzade[2], K Moshammer[2], R Fernandes[2], D Markus[2], M Geron[1], J Early[1] and H Grosshans[2]

[1] Queen's University, 123 Stranmillis Road, Belfast, UK
[2] Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

E-mail: `holger.grosshans@ptb.de`

Abstract. The accuracy of the experimental measurement of gas phase chemical kinetics related quantities using Jet Stirred Reactors (JSR) depends to a large degree on the homogeneity of the mixture inside the reactor. It is well-established that the mixing process in fluids is dominated by turbulent motions. Coherent turbulent structures are identified by applying the technique of Proper Orthogonal Decomposition (POD) based on previously performed highly-resolved large-eddy simulations. The structures of the highest energies are generated by the jets which inject fresh gases and in the wakes of the pipes leading to the injection nozzles. Furthermore, lower energetic regions were observed in the proximity of the impingement areas of the inlet jets on the surface of the spherical reactor chamber. The data provided herein contributes to the understanding of the flow dynamics in JSRs and aims to guide their future development in order to increase measurement accuracy.

1. Introduction

The experimental analysis of the kinetics of gas-phase reactions is usually carried out in facilities with generic geometry and idealized conditions. Examples of these facilities include rapid compression machines, shock tubes, static reactors, flow reactors, and Jet Stirred Reactors (JSR) [1]. The idealization of the latter device lies in the intent to generate a perfectly mixed and homogeneous composition. Various JSR concepts have been proposed which all promote the mixing of fresh and burnt gases inside the reactor by one or more jets. Thus, it is of utmost importance to carefully choose the JSR design in order to ensure an efficient mixing process is achieved.

However, the evaluation of the detailed flow inside the reactor can be difficult due to the limited optical accessibility in most experiments. In fact, available data sets are mostly limited to the measurement of the composition of the exhaust gases at the outlet, e.g. by laser absorption spectroscopy. One possibility to extend this evaluation is the injection of a tracer into the reactor and the subsequent measurement of the tracer gas concentration decay at the outlet [2]. The resulting tracer decay functions can be utilized to estimate the residence time distribution which is a commonly applied indicator to compare the mixing in a real reactor to an ideal one. Using this technique, Ayass et al. [3] evaluated the internal mixing in different JSR geometries by filling them initially with CO_2 followed by a sharp cut-off and a subsequent continuous flow of N_2.

However, several drawbacks are inherent in this methodology. First, the species initially present in the reactor and the tracer are naturally different and, therefore, usually characterized by different densities and viscosities. Insertion of a tracer itself represents a disturbance to the flow field, the contribution at which is difficult to quantify. Secondly, and probably more importantly, the tracer concentration is a single scalar at the outlet which is not sufficient to describe a complex three-dimensional flow field, with the underlying assumption that the composition at the outlet plane is perfectly mixed. Nevertheless, one can easily imagine a situation where the tracer and the initial species are separated, but their total concentration at the outlet nevertheless is equal to an ideal reactor.

The tracer decay technique has also been used in simulations of Esmaeelzade et al. [4, 5] characterizing the mixing in a JSR. These computations referred to a JSR design similar to the one of Dagaut et al. [6]. Four injectors are positioned in two perpendicular planes creating a circulating flow within the reactor. While primary motivation is to simulate the tracer decay due to the availability of comparable experimental data, it is expected that a more detailed understanding of the mechanisms of mixing would enable further improvements of the JSR design.

The enhancement of mixing by large-scale turbulence structures is a well-known phenomenon. Several post-processing algorithms have been proposed to identify turbulent structures including *Proper Orthogonal Decomposition* (POD) [7] and *Dynamic Mode Decomposition* (DMD) [8]. POD approximates the velocity fields obtained by simulations by a few linear combinations. These main components represent the coherent turbulent structures containing the highest energy. During the last decades both POD and DMD contributed significantly to the understanding of complex flows [9], in domains such as aeroacoustics [10], combustion instabilities [11] and reacting swirling flows [12].

The potential of POD has also been utilized by Hammad and Milanovic [13] to study the flow field inside a JSR. The vessel was of a cylindrical shape and the mixing was realized by a single nozzle of a variable position. They performed experiments and used Particle Image Velocimetry (PIV) to investigate the turbulent flow structures. POD analysis based on the PIV data provided valuable information concerning the most energetic coherent turbulent structures. However, since the geometry of the considered reactor was very different from the one previously simulated [4, 5], the results of Hammad and Milanovic [13] do not directly aid to understand the flow in the current vessel under investigation.

High-level post-processing techniques, such as POD have been applied to the flow field data inside a spherical JSR generated by Large-Eddy Simulations (LES) in the current study. The aim is to support the further advancement of the JSR design in order to obtain improved mixing. The numerical methodologies and the results obtained are discussed in the subsequent sections.

2. Flow-field simulations

The simulated reactors design follows the one by Dagaut et al. [6]. The spherical part of the vessel is 40 mm in diameter and the gas inside the reactor occupies a fixed volume of 32.8 cm^3. It is filled with CO_2 through four injection nozzles and contains an outlet of 10 mm diameter at the bottom. The flow is simulated for a time-span of 650 non-dimensional time units, where one unit corresponds to the ratio of the diameter of the sphere to the injection velocity. The simulation of the double time-span did not lead to any change of the resulting mean flow which demonstrates that a statistically steady-state flow was reached. Afterward, data for the POD analysis was collected for a time-span of 200 time units.

A temperature of 298 K was assumed for initial boundary conditions. For the pressure, atmospheric condition were considered at the outlet and zero-gradient at the walls. An unstructured mesh was generated and refined in relevant areas such as the walls, the inlets, and the outlet where higher flow gradients were expected. The flow field inside the reactor was computed using the *reactingFoam* solver of the *OpenFOAM* toolbox. A non-reactive flow of pure CO_2 is considered in the present study. Therefore, the relevant set of conservation equations is reduced to the mass and momentum equations. A spatial filter operator was applied to the governing equations, and the large-scale turbulent structures in the flow field were resolved on the grid by LES. The residual (sub-filter) scale stresses were modeled via the static Smagorinsky model [14]. Finally, we demonstrated the grid independency of the results by computing the present case on three different grid resolutions. For further details concerning the simulations, can be found in Refs. [4, 5].

3. Proper orthogonal decomposition (POD)

POD is a statistical procedure that is used in fluid mechanics to transform temporal realizations of a flow field into a reduced number of principal components (also termed *modes*) which represent coherent turbulent structures. In the Fourier decomposition, the modes are a-priori chosen to be sinusoidal while in POD the basis is empirical. The empirical basis is sought so to maximize the quantity [9]

$$\frac{\langle |(u,\phi)|^2 \rangle}{||\phi||^2} \tag{1}$$

where $\langle \cdot \rangle$ denotes the time or ensemble average, $||.||$ the norm and (u,ϕ) the inner product of a velocity component, u, and the basis, ϕ. For the computation of discretized 3-dimensional results the instantaneous flow field data is written in a single matrix $\boldsymbol{X}$ where each row corresponds to a grid point or velocity component and each column to a time instance. Through Sirovich's method of snapshots [15] the maximization of the quantity in equation (1) becomes an eigenvalue problem of a reduced size, namely

$$\boldsymbol{R}\boldsymbol{\phi}_j(\boldsymbol{x}) = \lambda_j \boldsymbol{\phi}_j(x) \tag{2}$$

where λ_j is the eigenvalue (i.e. kinetic energy) and $\boldsymbol{\phi}_j$ the basis of the j-th mode. Further, the autocorrelation matrix $\boldsymbol{R}$ is defined as $\boldsymbol{R} = \boldsymbol{X}\boldsymbol{X}^{\mathrm{T}}$.

The modes are ordered in a descending fashion according to their energy content, i.e. $\lambda_j > \lambda_{j+1}$. Moreover, since the variable of interest in the present study is velocity, the modes represent the decaying energetic content. The most energetic coherent structures are thus identified through the decomposition.

4. Results

The principle of operation of the JSR under consideration can be inferred from Figure 1 showing the time-averaged velocity magnitude in the x-z cross-section. This cross-section comprises the center-lines of two opposite located nozzles, one pointing upwards and other downwards. These orientations facilitate a vertical circumferential flow of fresh gases in counter-clockwise direction along the spherical surface of the reactor. In the same way, the other two nozzles establish a second circumferential flow. The second flow is horizontal, i.e., located in the x-y cross-section. As a result, both flows are perpendicular to each other and intersect at two points, namely at the extremities of the x-axis.

This choice of design results in the generation of coherent turbulent structures, analyzed by utilizing the POD technique. From identifying the energy content of the first 10 modes, it becomes evident that two modes dominate the spectra. More specifically, the first and second modes account for approximately 80 % of the total present turbulent kinetic energy. Modes 3 – 10 are each responsible for less than 4 % of the total kinetic energy. Therefore, the first two modes are of most interest for further discussion. The three dimensional representation of the isosurfaces of these modes is plotted in figure 2. The coherent structures exhibit a strongly non-symmetric pattern and are of a highly complex nature.

In order to obtain a more detailed insight, the fields corresponding to the first and second modes are given in figures 3 and 4, respectively. It is rather surprising that the turbulent structures of the highest kinetic energy are situated close to the nozzles and not close to the outer walls where the two circumferential flows are acting. More precisely, the structures can be differentiated according to their origin: First, one can identify toroidal shapes of the first mode attached to the orifices, e.g. visible at the upward pointing nozzle in figure 3. This is a common feature found in gas and liquid jets. In other words, the characteristics of the generated jets is the dominating mechanism for turbulent mixing in the JSR in the region close to the nozzles orifice. Second, highly energetic structures of both first and second modes can be observed close to the outer walls of the nozzle pipes. It is anticipated that this phenomenon relates to the turbulent wake of the gas flowing around the pipes. This hypothesis is supported by the fact that the local Reynolds number of the flow around the pipe, based on the outer pipe diameter and the inlet velocity, is about 100 000. This value is two orders of magnitude larger than the Reynolds number

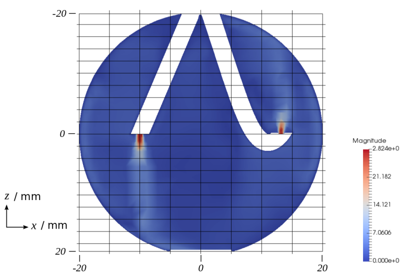

Figure 1. Time-averaged velocity magnitude (in m/s) in the x-z cross-section.

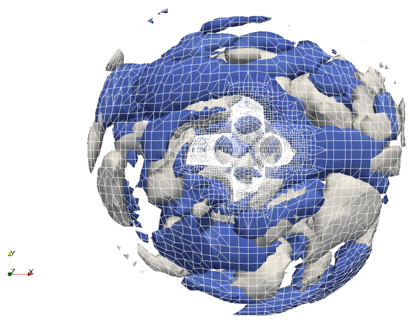

Figure 2. Isosurfaces related to POD modes 1 and 2 viewed from top.

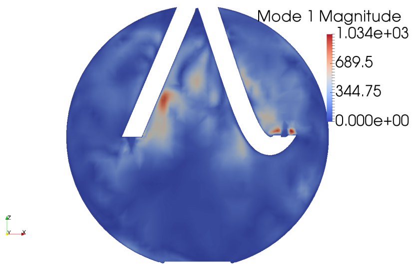

Figure 3. First POD mode in the x-z cross-section (arbitrary units).

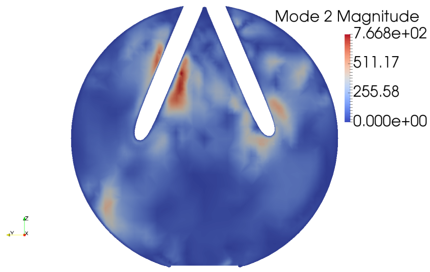

Figure 4. Second POD mode in the y-z cross-section (arbitrary units).

which was measured to be the onset of turbulence for the comparable case of the flow around a smooth, planar cylinder. From these observations, it is concluded that the solid surfaces inside the reactor do not represent an obstacle but rather enhance local turbulent mixing.

However, the interaction of the jets with the outer JSR walls also leads to turbulent structure development, albeit of a lower energetic content than the previously discussed types. These are mainly related to inclined impingement of the jets on the spherical surfaces. For example, the effect of the downward pointing jet can be seen in figure 4.

Finally,while POD facilitates the identification of multiple flow structures, their oscillating frequencies remain unknown. However, the frequencies can be an important factor in the analysis of mixing in reactors since the most energetic structures are not necessarily the most dynamic ones. Therefore, future DMD analysis will reveal whether this is the case in the considered JSR.

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